

## **Fast Dissociation in Core-Excited Ozone Studied by Resonant Auger Emission**

***S. L. Sorensen, L. Rosenqvist, K. Wiesner, A. Naves de Brito, M. Bassler, R. Feifel, I. Hjelte, C. Miron, H. Wang, M. N. Piancastelli, O. Bjorneholm and S. Svensson***

*Department of Synchrotron Radiation Research, Institute of Physics, University of Lund, Box 118,  
S-221 00 Lund, SWEDEN*

*Department of Physics, Uppsala University, Box 530, S-751 21 Uppsala, SWEDEN*

*Laboratorio Nacional de Luz Sincrotron, Box 6192 CEP 13083-970 Campinas SP BRAZIL*

*Department of Chemical Sciences and Technologies, University "Tor Vergata", I-00133 Rome,  
ITALY*

The somewhat unique chemical composition of the highly reactive ozone molecule makes it an ideal candidate for spectroscopic studies. The central oxygen atom has a binding energy approximately 4 eV greater than that of the terminal oxygen atoms, making site-selective studies using resonant excitation methods possible. Here we present Auger electron spectra from emission after excitation to repulsive core-excited electronic states of  $\sigma$  symmetry in ozone. The decay spectra are analyzed in terms of Auger decay and fast dissociation. The electronic states seen in the Auger spectrum reflect the fate of the core hole; molecular Auger lines arise from decay within the bonding region of the final states while dissociation leads to Auger emission at energies corresponding to transitions between atomic levels. By application of the site-selective excitation, the resonant Raman Auger conditions and angle-resolved electron and ion emission measurements the dissociation is confirmed.

In this work a study of excitation of localized core electrons from both the terminal and the central oxygen atoms to highly repulsive states in ozone is presented. We find clear evidence of dissociation directly from the terminal oxygen core-excited state and we find that the measured dissociation products always consist of a core-excited oxygen atom and a ground state oxygen molecule. The decay from the two chemically-shifted oxygen atoms leads to dramatically different final-state spectra. The origin of these differences is discussed partly in reference to electron-ion coincidence measurements made at the same resonant energies.

In addition, the energy shift of the atomic Auger electron which reflects the kinetic energy of the atomic fragment upon dissociation is analyzed. Upper and lower bounds on the kinetic energy released upon dissociation are extracted from this data and from a Born-Haber cycle. The possibility for the molecular fragment to carry energy in the form of internal vibrations accounts for part of the large spread between these values, but the former method depends upon accurate measurement of the maximum kinetic energy imparted on an electron. The accuracy of this method is limited mainly by the range of angles over which the dissociation can take place.